XPDF

A Dedicated X-ray PDF Beamline
Phase III Beamline Proposal

A proposal prepared for the SAC January 2011

Acknowledgments

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The working group gratefully acknowledges the valuable contribution of the following individuals, who participated in the XPDF workshop held at Diamond House on 13 January 2011, and/or who provided direct input into the preparation of this proposal through other means.

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Please note that the list of contributors of letters of support (distinct to the list above) is given separately on Pages 23–25 of this document.

1. Summary

Our vision for XPDF is straightforward: to build an instrument that measures X-ray pair distribution function (PDF) data of the highest quality possible at DLS, servicing the very large number of UK research groups whose work relies on understanding local structure in materials.

Never before has the importance of understanding local structure been so clear in so many disciplines: in the development of advanced materials for energy applications, for the digital economy, for the pharmaceutics and health industries, and for fundamental sciences from chemistry to physics to earth sciences. The ability to measure X-ray PDF data at Diamond is crucially needed because the technique is the *only* truly quantitative probe of local structure correlations in materials. Whereas the sensitivity of "traditional" local structure techniques—such as EXAFS and NMR—is dominated by nearest-neighbour interactions, the PDF measures structural correlations across all length scales in a single experiment. Indeed the accuracy with which latest-generation instruments at spallation neutron sources and X-ray synchrotrons can measure the PDF, together with an increasing sophistication in the analysis methods, has seen a step-change in the significance of the scientific questions addressed using the technique. As the UK community using PDF techniques in their research continues to grow and diversify, there is an increasing desire for high-throughput measurements, a more diverse range of materials to be studied, and varied sample environments and measurement timescales. The corresponding need to work with small sample sizes and over short timescales means these studies demand a UK synchrotron X-ray PDF facility.

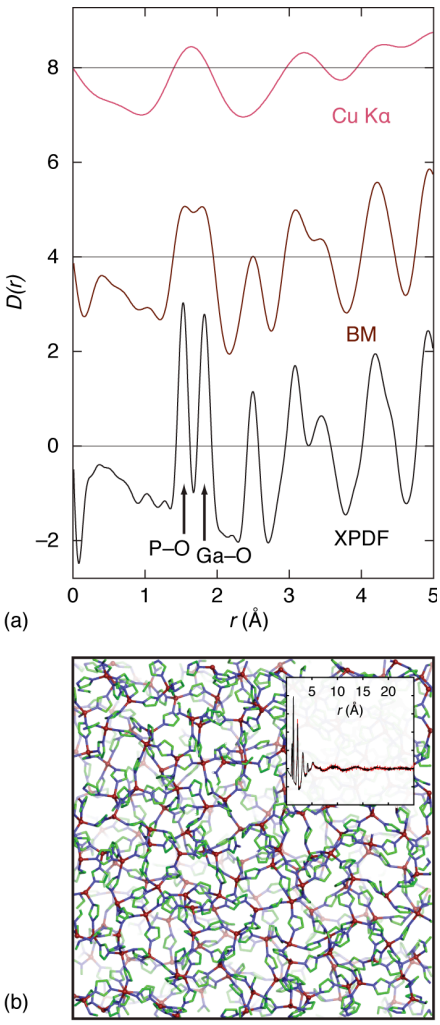
The absence of an X-ray PDF instrument at Diamond is already conspicuous. Diamond is the right place for such an instrument because (i) it offers a stable source of X-rays of sufficiently high energy for PDF measurements, (ii) there is the right expertise to make the facility successful, (iii) having X-ray *and* neutron PDF facilities on the same campus offers a synergistic relationship that increases value both at DLS and at ISIS, and (iv) there is strong complementarity between PDF capability and the existing portfolio of Diamond beamlines. PDF studies require very careful measurement because they rely on accurate determination of weak diffuse scattering features that would otherwise be treated as background; it is no accident that many more beamlines would claim to be capable of measuring PDF data than have proven to be capable of producing high-profile PDF work. Our focus on a *dedicated* PDF beamline is to ensure a design and mode of operation that will produce world-class PDF data of genuine use to the research community.

We propose to build XPDF as a side-station to the existing I15 beamline, making cost-effective use of the existing I15 superconducting wiggler to provide the high-energy X-ray beam needed for PDF measurements. The aforementioned sensitivity of PDF measurements to instrument background, the need to work at high energies, and the space limitations as a side-station have provided us with very stringent constraints on instrument design. In fact we have used these constraints to focus our proposal on its core objective of delivering reliable X-ray PDF data. The XPDF design allows for the different sample environments and data collection modes required to accommodate the vast majority of science interests of the anticipated user community but does so without compromising the central need for straightforward, robust and high-quality X-ray PDF measurement capabilities. Our plans for XPDF will ensure that the UK remains at the forefront of this emerging and important field.

2. Scientific Case

Of all the experimental probes of local structure, PDF techniques benefit from the unique advantage that the PDF is a directly-measurable histogram of interatomic distances. Because it is quantitative, it can be used for *local* structure refinement in much the same way as Bragg diffraction patterns are used for *average* structure refinement. The immense scientific insight this can provide is rapidly gaining notice: it means PDF methods can be used to produce realistic atomic-scale models of the local structure in materials—crystalline, nanocrystalline, amorphous or fluid. Indeed, for glasses and fluids, the PDF has always been the primary approach to understanding atomic structure, but increasingly PDF methods are being used to provide unique insight into the properties of crystalline materials. There is a growing realisation that for many important classes of crystalline material the instantaneous local structure is significantly different from the average. Surprisingly often it is this difference that is so crucial to the physical and chemical properties of these materials.

Experimentally, the PDF is measured as the Fourier transform of the X-ray or neutron scattering function taken to large maximum values of the scattering vector Q. These measurements present a number of challenges. Unlike traditional crystallography, where the focus is on extraction of Bragg peaks, it is critical to be able to minimise and measure accurately the background scattering. This directly impacts on the design of the instrument, including the way in which sample environment control is incorporated into the design. It is essential to measure to maximum values of Q that far exceed those traditionally used in crystallography, because the maximum value directly determines the best resolution possible in determination of interatomic distances (see figure). The situation is made more difficult for X-ray PDF measurements by the unavoidable loss of scattering intensity at high-Q arising from the fall-off of the X-ray form factors, compounded further by the increasingly dominant contribution of Compton scattering that degrades the signal-to-background ratio in the same region of the scattering pattern. Diamond offers the combination of high X-ray energies (hence wide Q range) and high flux (hence accurate measurements at high-Q) that is crucial for measuring accurate PDF data; XPDF is configured for an operating Q_{max} value of 44 Å^{-1}. But it is equally important that the experimental requirements necessary for low backgrounds



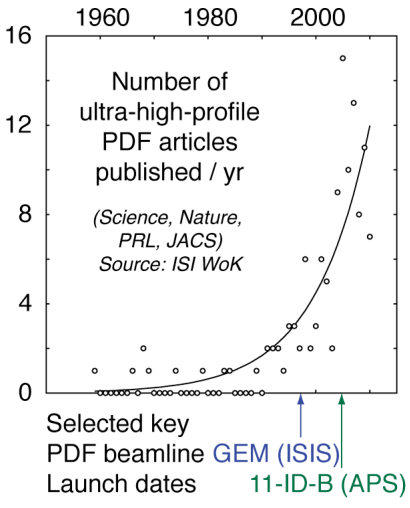
(a) The effect of X-ray energy on PDF resolution: The P–O and Ga–O bond lengths in $GaPO_4$ are indistinguishable using a laboratory CuKα source (top), barely distinguishable if XPDF were to use a bending magnet (middle), and clearly separable using the medium-energy (65 keV) configuration of XPDF as a side-station on I15 (bottom). (b) An illustration of the structural modelling possible using PDF techniques—in this case for an amorphous metal–organic framework [1].

and robust data normalisation are not underestimated; the community experience is that this is only practicable at dedicated PDF facilities, and hence the imperative behind our XPDF bid.

The growing appreciation of the potential of PDF within the broader scientific community is reflected in the very high oversubscription rates reported for the few dedicated X-ray PDF beamlines that currently exist (*e.g.* 4–5× for the APS X-ray PDF beamline 11-ID-B). This increased uptake of the technique is having a number of important consequences of relevance to this XPDF proposal:

1. We are in a position where PDF measurements are being performed using an increasingly broad and ambitious range of sample environments and data collection modes. Notably this includes sub-second PDF measurements (now possible at rates of *ca* 30 Hz) for time-resolved studies [2] and differential PDF measurements for multicomponent systems such as nanoparticle deposits on solid substrates [3]. Within firm reach is the application of PDF measurements to studying correlations in thin-film samples, the use of small beam widths to probe correlations between nano- and macro-structure in materials, and real-time *in situ* measurements of chemical processes occurring in complex reaction media.
2. The relevant detector technology is improving rapidly. We have already seen vast increases in the size and readout speed of 2D "image plate" detectors. Over the next 5 years, we understand that high-performance 1D strip detectors suitable for PDF measurements will become available. These will offer the combination of fast read-out times with a 2θ coverage (and hence Q range) that is many times greater than that offered by the existing 2D detectors.
3. Both the variety and capability of software for PDF analysis are increasing. Normalisation of X-ray PDF data and extraction of straightforward local structure information—bond lengths, coordination numbers, particle sizes—has largely been automated through software such as PDFGUI [4] and GUDRUN [5]. At the other extreme of modelling complexity, it is now viable to refine large atomistic models of material structure from X-ray PDF data using *e.g.* RMCProfile [6] and/or EPSR [7]. Importantly for XPDF much of this software development has been undertaken within the UK community and so there is an enormous body of expertise on which to draw when developing software to process data collected at XPDF.

On the following pages, we outline representative topics across a broad range of science fields where the XPDF beamline would be likely to enable significant breakthroughs. These research areas span all the key priority themes of materials development: energy (battery materials, carbon capture via gas sorption, hydrogen storage, catalysts); health (pharmaceuticals, biomaterials); digital economy (digital storage media, electronics materials and semiconductor components, display materials, plastic electronics). Where appropriate, we also draw attention to areas that are likely to interface directly with key R&D areas for UK industry.



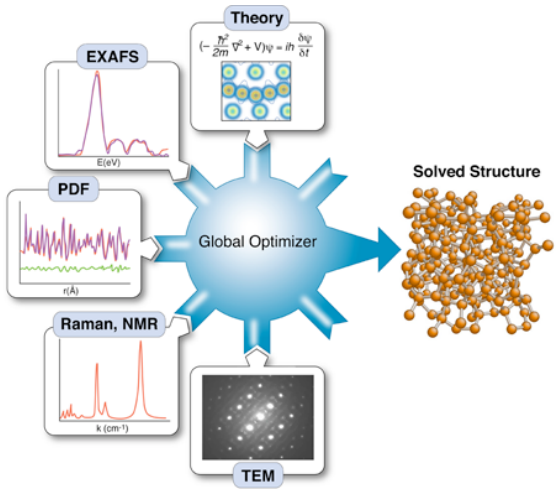
One common theme that emerges very clearly is that PDF measurements—wherever they are performed—will not only provide important insight into new fields as they emerge, but are capable

of driving new and important science that would otherwise not be achieved. Studies in which PDF measurements have played a key role are appearing increasingly often in journals of the very highest calibre (see graph on the previous page); indeed we are aware of two papers published in *Science* and *Nature Materials* in the last four weeks alone [8,9].

So why is it that XPDF will drive world-leading new science at Diamond?

Understanding local structure is fundamentally important for basic and applied science alike. Across fields as diverse as biomineralisation and condensed matter physics, in industrial applications and in basic research, the science of interest involves understanding chemical and physical interactions that occur on the atomic scale—be it, for example, to watch and control catalytic mechanisms, to investigate adsorption in porous materials, or to characterise the structural rearrangements that accompany electron flow in battery materials. All these processes are affected by the local environments of individual atoms.

PDF methods are the most sophisticated tool available for characterising local structure. Because the PDF is quantitative it is unique among experimental local structure probes in its ability to *drive* the refinement of structural models. Moreover the models obtained are inherently consistent over different length scales (*e.g.* with long-range periodicity from diffraction) and other experimental and theoretical information can be readily included in the refinement process (see graphic).



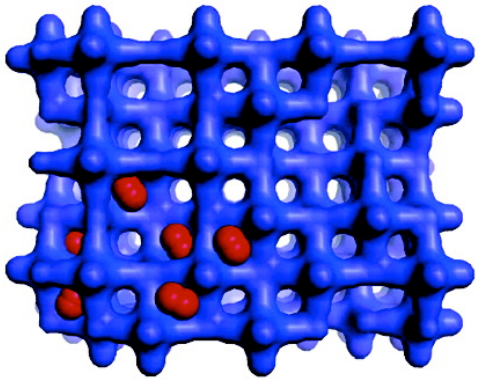
PDF techniques play a central role in emerging paradigms for the determination of complex structures— such as nanoparticles, disordered materials and multicomponent phases [10,11].

XPDF complements rather than replicates the existing portfolio of instruments at Diamond. XPDF will be the first dedicated X-ray PDF instrument of its kind in Europe. It will interface directly with the current EXAFS and powder/single-crystal diffraction capabilities of Diamond, and operate synergistically with the scientific programmes of the extreme conditions and engineering beamlines. There is a strong and rapidly growing UK community looking to use X-ray PDF measurements in their research, guaranteeing a healthy oversubscription rate even in the early days of XPDF.

XPDF is focussed on doing one thing and doing it well. Being a dedicated instrument means that it is possible to optimise all aspects of instrument design to enable measurement of the highest quality PDF data possible at Diamond. We are especially mindful that XPDF will be used by a community that is largely new to the technique. It is the general experience that whenever PDF is not the core focus of a beamline, data reduction and treatment is not straightforward and the non-expert user is quickly discouraged. Instead our goal is that XPDF produces usable, robust PDF data obtained with the minimum of fuss: this will be the key to driving new science as quickly as possible.

Chemistry and Catalysis

One of the most intensively-pursued research areas in chemistry is the design of functional porous compounds with applications in gas storage (*e.g.* for H_2, CO_2) and catalysis. The key challenges in this field centre around characterisation and rationalisation of the interaction between guest species and the host material into which they are introduced. This includes, for example, establishing the role of open metal sites in gas storage within metal–organic frameworks [12]; "gating" mechanisms for hysteretic gas uptake [13]; and the method of guest activation during catalysis [14].



Nitrogen adsorption sites in a cubic "Prussian Blue"-type framework material determined using differential PDF measurements. Figure taken from Ref. [15].

In all these cases, "traditional" crystallographic techniques are not helpful because (i) the stoichiometry of guest uptake is often low so that not all adsorption sites are occupied, (ii) the positions of these molecules are usually disordered over very many sites, and (iii) the molecular orientation (and hence the chemical nature of the host-guest interaction) is usually not known. "Differential PDF" measurements [15,16], which contrast the PDFs of guest-free and loaded states, provide direct information about the host-guest interactions. X-rays are particularly suited to such studies because of the small sample volumes, and because time-resolved X-ray PDF measurements can be performed to provide kinetic information about the sorption and desorption processes.

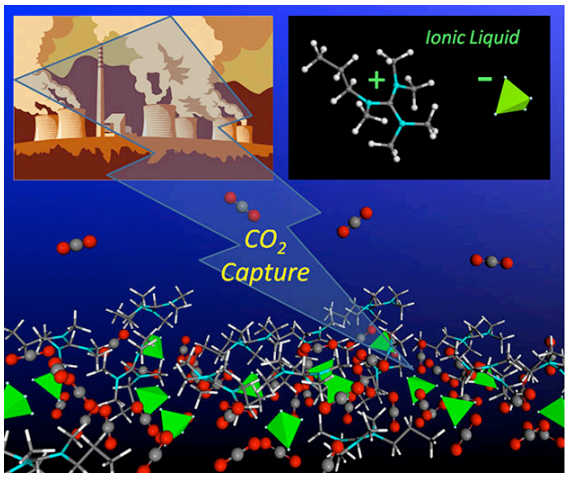
For the catalysis community, time-resolved X-ray PDF measurements will be massively important because they offer a means of "watching" *in situ* the structural transformations that accompany catalytic processes. Indeed the industry makes use of many disordered or "nanostructured" material types that are inherently poorly suited to traditional diffraction studies but ideal for characterisation using PDF: nanoparticles, functionalised zeolites, thin films and layered materials.

Rapid PDF acquisition provides a uniquely valuable window into the fundamental processes of nucleation and growth by documenting the evolution of different local correlations as a function of time [2]. This is key in the design of functionalised nanoparticles where it is crucial to control the distribution of particle size and shape obtained at different stages during synthesis. Likewise it is commonly found that growth of crystalline solids proceeds via a number of different intermediate states—including amorphous and poorly crystalline forms—and by being able to correlate directly the changes in local and average structure that occur, X-ray PDF methods offer a means of probing the underlying mechanisms that govern these solid-state transformations [17].

Unprecedented insight into the more general phenomenology of structural phase transitions is attainable using PDF measurements. This includes understanding how the interaction between local distortions precipitates structural transitions with changes in *e.g.* chemical composition, temperature and pressure. *In situ* experiments would allow the contrasting mechanisms of topotactic and reconstructive transformations in key oxide families to be compared on a local scale and a microscopic understanding of intercalation processes in layered materials to be developed.

Materials for Energy Applications

In addition to the development of gas-storage materials flagged in the previous section, one important immediate challenge in the field of energy materials is to develop battery technologies that will enable organic fuels to be phased out from transport, with subsequent benefits for batteries with enhanced life for mobile electronics. Battery processes involve the transport of ions through disordered materials, with time-dependent changes through the charge/discharge cycle and through the battery life. The changes in structure involved (which extend beyond the first coordination shell accessible using EXAFS/NMR) must be understood on a local scale, and PDF measurements are critical for this. XPDF will allow users to work with small samples for parametric studies (*e.g.* materials with different charge/discharge histories), and to perform *in situ* time-resolved studies.



Ionic liquids are capable of selectively separating greenhouse gases such as CO_2 from emission sources; the effectiveness of different solvents is governed by local interactions between the solvent and CO_2 molecules—interactions to which PDF measurements are especially sensitive [18].

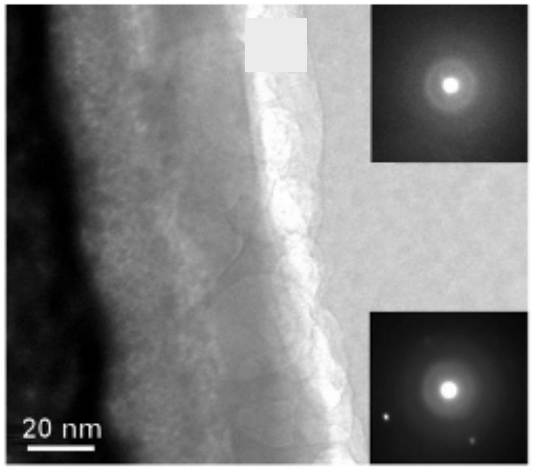
The development of increasingly efficient fuel cells relies on understanding the electrochemical processes that occur during cell operation. These are inherently difficult to study on the atomic scale: there are multiple oxidation states present, complex diffusion processes occurring and noncrystalline phases present. One important challenge for the future of XPDF will be the development of sufficiently robust *in situ* PDF measurement protocols that will facilitate development of realist atomic-scale structural models of such processes.

Long-term storage of nuclear waste relies on the development of materials that resist leaching after sustained structural degradation through radioactive decay. Because the structural disorder introduced during decay involves the 1–10 nm length scale, PDF measurements are one of the few experimental techniques sensitive to the structural changes involved. The key question in the field is to establish which structural components of the host material most effectively reduce the extent of damage—the answer is needed so that informed material design might maximise the density and lifetime of nuclear waste storage. The combination of PDF measurement and atomistic modelling currently being employed elsewhere would provide the ideal means of answering this question.

Ionic liquids are a broad family of structurally mobile salt phases with a number of key energy-related applications: in carbon dioxide capture, nuclear fuel reprocessing, solar energy, and as battery electrolytes. Understanding local structure/property relationships in this family is key to the continued development and commercial exploitation of functional ionic liquids. The problem faced by the relevant community is that the structural variations that occur during solvation and flow extend over the 10–50 Å length scale, which is inaccessible using EXAFS and NMR. To date there has been a heavy reliance on simulation data but by characterising local structure correlations XPDF will provide valuable experimental constraints on the development of these models.

Materials for the Digital Economy

Amorphous transparent conducting oxides (TCOs) are a family of materials that have attracted enormous interest for their potential as transparent thin-film transistors, as organic light-emitting diodes and as the key candidates in the emerging class of transparent electronic devices in large area flexible displays and circuits [19]. It is thought that the structures of these materials are related to that of their crystalline counterparts, and models for their electronic properties are now being put forward on this hypothesis [20]. But the absence of long-range periodic structure means that XPDF will prove crucial in providing a firm structural basis for understanding transport properties of this important family.



Amorphous transparent conducting oxide (TCO) films have superior conductivity and optical properties to their crystalline counterparts but the reason for this difference—and hence how best to exploit it—is not understood [20].

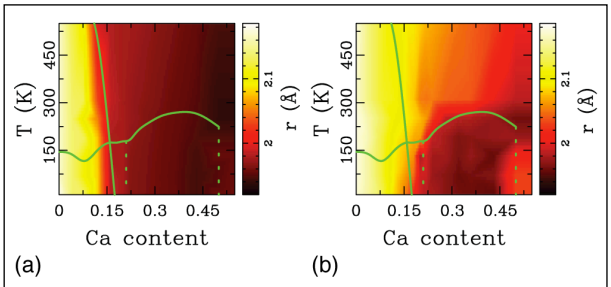
As X-ray PDF measurements continue to develop, it will become feasible to study local structure in thin-film samples. The current difficulty faced is the low sample-to-substrate ratio and hence the dominant scattering of the substrate itself. Differential PDF measurements exploit the high X-ray flux obtainable at synchrotron sources in order to obtain sufficient counting statistics that the substrate scattering can be subtracted and the sample-only PDF obtained. One relevant area where such studies will prove especially valuable is the structural characterisation and development of thin-film ferroelectric materials, which are finding application in a diverse range of fields: as components in microwave circuits, semiconductor devices and visible-light photovoltaic devices. The respective bulk ferroelectric materials (discussed in more detail in the next section) are themselves already well suited to PDF studies; but it is the additional local distortions imposed by processing as thin films that are especially important to characterise, for which X-ray PDF data will be essential.

Defect sites and nanoscale regions of disorder in dilute magnetic semiconductors have been shown to be a crucial structural aspect in the development of spintronic materials [21]. In developing computational models of spin transport in these systems the nature of this disorder is of fundamental importance: this is an obvious area where PDF measurements again have a key role to play.

Digital storage media applied in DVD-RAM technology exploit the rapid kinetics of reversible optical switching between crystalline and amorphous forms of chalcogenide compounds. The timescales involved hint at the importance of "crystal-like" domains that persist in the amorphous state, and PDF methods are starting to play an important role in providing the structural understanding necessary to optimise the chemistry of these materials (*i.e.* which chemical components facilitate ordering and which encourage amorphisation [9]). Very recently, a number of phase change chalcogenides have also been shown to produce very strong nonlinear optic effects [22]. This behaviour implies the persistence of local noncentrosymmetry across the crystal-to-amorphous transition—and indeed PDF measurements are already starting to be applied to understand this effect.

Physics of Condensed Phases

Many of the most important material families in condensed matter physics—multiferroics, colossal magnetoresistance (CMR) manganites, oxide high-T_c superconductors—involve atoms with variable valence states. Because ionic size and covalent bond lengths change with valence, local stresses and structural relaxation over short length scales are recurring features in all these materials. Local distortions are made all the more important by local symmetry lowering in Jahn Teller systems, for which geometric correlation between distorted metal coordination polyhedra is widely considered to play a key role in producing phenomena such as CMR. These local distortions and the medium-range correlations between them can be probed with high accuracy using PDF studies; indeed PDF studies have already led to a number of high-profile results in this general field [23]. The real strength of the technique is its ability not only to probe the nearest-neighbour distances within these materials, but also to provide constraints on how local distortions are correlated throughout the corresponding structure. What is now clear is that the local structure—and not the average—is more strongly coupled to key electronic properties (see figure); this serves to underscore the importance of PDF measurements in establishing structure/property relationships in these important families.



Temperature/composition-induced variations in Mn–O bond lengths obtained from (a) average structure analysis are not sensitive to electronic changes within the CMR family $La_xCa_{1-x}MnO_3$; however the equivalent values determined (b) using PDF measurements correlate well to the electronic phase diagram [23].

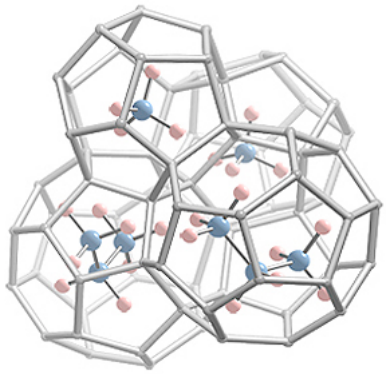
The properties of relaxor ferroelectric structures are determined by chemical disorder, which again leads to local stresses and relaxation on the 1–10 nm lenth scale. Being sensitive to these structural distortions, XPDF will allow experiment-driven modelling of polar nanoregion (PNR) formation in these materials [24]; moreover, the continued development of *in situ* PDF measurements will allow for the first direct observation of variation in PNR habit under changes in applied field.

The highly attractive electronic and mechanical properties of graphene, fullerenes and inorganic nanotubes have seen the emergence of a high-profile active community interested in understanding and exploiting the physics of "nanostructured" systems. However, structural characterisation of these materials is inherently difficult because few are obtainable in crystalline form. The development of PDF-based techniques for structure solution of these materials is seen as one of the most promising and important advances in the area, and XPDF will play an important role in its future.

PDF measurements have always played a key role in structural studies of highly disordered materials such as liquids and glasses. An increased diversity and complexity of relevant systems has meant that interest in this field is stronger now than ever before: complex ionic and molecular fluids, new metallic, ionic and molecular glasses, and even glasslike phases of metal–organic frameworks [1]. The absence of long-range periodicity in all these materials leaves PDF as the method of choice for determining their structure and for studying phenomena such as liquid–liquid phase transitions and the amorphisation process itself. In all cases, one expects (and finds) structural correlations that extend well beyond the first coordination sphere: hence the desirability of PDF.

Earth & Environmental Sciences

Whilst processes in Earth and Environmental Sciences are typically thought of in length scales from the metre to thousands of kilometres, the properties of environmental and earth materials are determined by interactions and structure on the atomic scale. Methane hydrate clathrates (MHCs) are a topical example because of their involvement in the recent Deepwater Horizon oil accident. MHCs consist of a cagelike network formed by water molecules with methane molecules occupying the cage cavities in a disordered arrangement (see figure). There are considerable fears that global warming may lead to their melting and subsequent release of methane. Our understanding of the stability of MHCs depends on understanding the details of the structure, which is made difficult by the large degree of structural disorder present. The simulation and NMR studies performed to date have left important questions unanswered: how the occupancy of one cage affects that of its neighbours; what the decomposition pathway involves; whether particular cage structures are more resistant to decomposition than others. These are the sorts of questions for which XPDF will be well posed to provide answers: the high X-ray flux and possibility of time-resolved measurements will allow local structure correlations to be measured *in situ* as samples are synthesised and allowed to decompose in pressure cells.



Methane hydrate clathrates are highly disordered materials of key environmental importance whose formation and decomposition pathways are ideally suited to X-ray PDF studies [25].

Clay minerals have important applications in geological waste containment, water storage and heavy metal sequestration. Most clays are poorly crystalline due to their strongly variable chemical compositions, variable water content and lamellar structures. The important science of clays centres around their physical properties on the atomic scale; for example, the structure of the interlayer water and host/guest interactions with adsorbed species. Together with on-site EXAFS studies, XPDF will play an important role in characterising local structure in these phases.

Natural hazards such as earthquakes and volcanoes are determined by the structural and mechanical properties of solid and fluid silicates. These materials typically contain networks of linked SiO_4 and AlO_4 tetrahedra, and local structure probes are essential because there is considerable flexibility of these networks that gives rise to dynamic disorder. X-ray PDF measurements provide the ideal probe of local silicon and aluminium environments; moreover, with the availability of laser heating X-ray PDF measurements may provide an attractive route to study local structure in silicate fluids.

A number of “nanostructured” materials assume important environmental roles, and PDF measurements will be necessary to determine structure–property correlations in these systems. Examples include nanomaterials generated as fine-scale dust in volcanoes (“volcanic ash”), the role of nanomaterials in the atmosphere to nucleate water droplets, and key mineral phases such as ferrihydrite, which is also used in biological systems as a natural store of iron [26]. Time-dependent PDF measurements will find application in studying nanoparticle growth, which has implications for their geological and biological roles alike.

Pharmaceutics & Biomaterials for Healthcare

Many of the drugs emerging from contemporary drug discovery programmes in areas including heart disease, cancer and infectious diseases, show very low aqueous solubility and consequently may not be suitable for oral administration in preferred tablet or capsule forms. Hence the formation, stability and properties of amorphous solids are of increasing interest to the pharmaceutical industry, in particular as they can confer increased aqueous solubility to drug compounds compared with traditionally preferred crystalline form [27]. However exploiting the amorphous form in a regulated medicine presents considerable scientific challenges that include: (i) phase identification—the lack of quantitative methods for structural identification presents difficulty during development and for IP protection and manufacturing quality control; (ii) ensuring stability—the thermodynamically metastable amorphous form will often revert to the less soluble crystalline state, altering the performance of the medicine.

Preparing amorphous forms of pharmaceutical ingredients is one of the key strategies being employed to improve bioavailability of insoluble compounds. XPDF will offer a uniquely robust method of characterising structure in these next-generation pharmaceutics. Image taken from ref. [28].

PDF analysis of local packing in amorphous and nanocrystalline drugs will transform our capability to monitor, to control and ultimately to design non-crystalline molecular materials in order that they can be exploited in novel products. XPDF offers a quantitative means of characterising local structure in amorphous and nanocrystalline drug materials. This includes "fingerprinting" non-crystalline forms to provide unambiguous identification and to monitor the impact of processing on solid form [29]. Also, utilising PDF analysis to track structural changes as a function of time, temperature and %R.H. will shed light on the relationship between molecular structure, local packing, intermolecular interactions and key physical properties including stability. Indeed, it is particularly exciting to consider the prospect that PDF analysis combined with appropriate data analysis and modelling capabilities would offer the prospect of solving the structures of amorphous molecular materials. Such studies would also allow the evolution of structure associated with crystallisation to be revealed. In addition to providing new insights into the fundamental processes of nucleation and growth, the research would establish a structural rationale for approaches to stabilise amorphous drug forms, for example, using polymer dispersions [30,31].

In addition to pharmaceuticals, there are many important biomaterials whose activities are related to their amorphous structure. For example, in addition to being a natural precursor for bone formation, amorphous calcium phosphate is used in dental treatments to remineralise tooth enamel as well as in cement composites used in *e.g.* hip replacements. Recent PDF studies of the biomineralisation precursor amorphous calcium carbonate have revealed how the structures of amorphous salts can be remarkably different from those of their crystalline counterparts (hence the importance of PDF) [32]. Understanding these differences is an area of sustained and fundamental interest. The role of local structure in bioactive silicate glasses to promote bone regeneration [33] receives similar attention having widespread application as implant materials to accelerate healing of damaged bones.

Complementarity

For many of these science areas—particularly for those involving small sample sizes, complex sample environments or time-dependent measurements—X-ray PDF measurements are without question the experimental probe of choice. There will be many cases, however, where neutron PDF measurements would provide valuable additional information. The differences in atomic scattering factors for X-rays and neutrons mean that the two radiation sources are sensitive in different ways to different atom types and this ameliorates to some extent the inherent lack of element specificity in the technique. In this sense, X-ray PDF techniques are complementary to neutrons rather than being competitive. As the complexity of systems being studied using PDF methods increases, we fully expect that the use of both types of radiation will become increasingly important; indeed much of the highest-profile PDF work already exploits both techniques in tandem.

The local structure information contained within EXAFS and NMR provides additional element-specific information—even if only for the first coordination shell of probe nuclei. For science questions where a particular atom type is present only in very small concentrations, such experiments will also complement the bulk structural modelling driven by XPDF. While it has historically often been difficult to resolve EXAFS and NMR results with the average structure models obtained using traditional crystallography, contemporary PDF refinement methods offer a self-consistent approach to studying structure on local-, medium- and long-range scales by utilising simultaneously the constraints provided by many types of experimental data. We see XPDF as playing an important role within the structural characterisation portfolio at Diamond by bridging the gap, as it were, between the EXAFS and diffraction capabilities already present.

There are also significant advantages in having an X-ray PDF instrument located on the same site as the ISIS neutron facility. The strength of PDF instrumentation at ISIS has played no small role in the development of international leadership in this area within the UK research community, including the development of flagship computer codes for PDF analysis (RMCProfile [6], EPSR [7]). This leadership will be exploited and will be significantly enhanced by the provision of a PDF instrument at Diamond. At the present time, UK PDF work with X-ray beams is being exported to overseas facilities, such as SPring-8 and the APS. There is of course no inherent problem with international collaboration, but a reliance on international facilities has important consequences. For example, whereas at the APS beamline 11-ID-B there has been rapid uptake of the technique by a broad community of users who are new to PDF, the present UK user community (who are forced to travel for X-ray PDF measurements) is dominated by groups who are specialist PDF users. A similar effect is observed at the ESRF, where the absence of a dedicated X-ray PDF beamline has almost certainly deterred non-specialist users who are reluctant to demand the instrument reconfiguration necessary in order to perform high-quality PDF measurements.

Community Development

One of the most enjoyable aspects of preparing this case for support has been the very clear indication that XPDF will act as a strong driver for the development of the UK PDF community beyond specialist users. We have seen this, for example, in the eagerness with which new potential users participated in the XPDF workshop; it is clear in the large number of letters of support from industry and academia alike; another good indicator is the popularity of the PDF workshop held at the

British Crystallography Association Spring meeting, which attracts more than 50 participants despite the absence of a UK X-ray PDF facility. XPDF is crucial to the growth of this nascent community. We see this working in three ways. First, healthy oversubscription rates to XPDF will help ensure the highest-profile science is performed at the beamline, which in turn further stimulates a growing community. Second, dedicated beamlines are proven to act as a magnet and flag for growing communities. Third, a dedicated PDF beamline will require staff—ideally with a Principle Beamline Scientist—who will develop expertise in both running PDF experiments and in using and developing PDF analysis software, and be able to support the community. In this regard we note that the co-location of Diamond with ISIS means that synergies between the beamline scientists will lead to opportunities in development of analysis software that are not possible elsewhere.

The sense in which XPDF is key to driving *future* scientific discovery in the UK—beyond the state of the art—is particularly exciting. To quote one letter of support, which is typical of many:

> *"Establishment of a dedicated beamline at Diamond would provide a UK focus for developments that would enable new materials science and support a large number of researchers including non-experts (in PDF) such as myself who are now recognising the impact that this technique can have on their future research."*

But perhaps the most striking aspect of the growing PDF community is the breadth of research disciplines it spans—Chemistry, Physics, Materials, Engineering, Geology, Pharmacology, and Biological Sciences—a key indicator of the scope of impact that XPDF will have on UK research.

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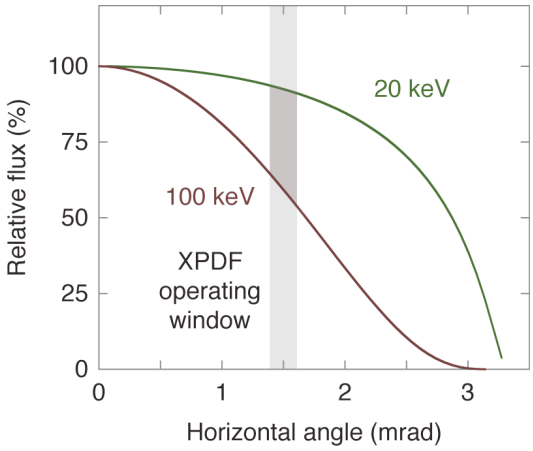
3. Beamline Requirements

Internationally competitive X-ray PDF measurements require the use of short wavelength (high energy) radiation, delivered to the sample with high flux and with moderate spectral purity. The short wavelengths and high flux are required to facilitate the measurement of the structure factor to large values of the momentum transfer, Q, with sufficient counting statistics to compensate for the X-ray form factor driven decrease in scattering intensity. Moderate spectral purity is required to resolve closely spaced Bragg scattering features in the signals of crystalline or partially crystalline systems. The baseline characteristics of the proposed beamline thus require the X-ray source to deliver radiation with wavelengths < 0.3 Å, which corresponds to photon energies above 40 keV, and with photon fluxes of *ca* 10^{11}–10^{12} photons/s, with a spectral purity of $\Delta\lambda/\lambda$ ($\Delta E/E$) = 10^{-3} or better.



The relative spectral flux of the I15 superconducting multipole wiggler as a function of viewing angle and beam energy. The primary beamline views the centre of the fan (±0.25 mrad) which allows a side station to receive a similar fraction of the fan with a beam centre offset by ±1.5 mrad.

The I15 superconducting multipole wiggler provides an ideal source for XPDF. It delivers a broad fan (±3 mrad) of high energy, high intensity X-ray radiation that allows construction of a side station each side of the main beamline. A side station taking radiation at 40–80 keV from a beam offset by 1.5 mrad would receive photon fluxes in the region of 70–80% of the primary peak flux. Preliminary calculations show that an instrument accepting a beam from this source, collimated by a 100 µrad × 100 µrad aperture and monochromatised using a standard +/– double crystal monochromator configuration, could expect a photon flux and spectral resolution at the sample to be in the range given in the following table.

Si crystal cut	Energy (keV)	Wavelength (Å)	Flux (photons/s)	Resolution ($\Delta E/E$)	Q_{max} (Å^{-1})
111	40.0	0.31	2×10^{12}	2×10^{-3}	41 (23)
220	65.3	0.19	4×10^{11}	2×10^{-3}	66 (38)
311	76.6	0.16	1×10^{11}	2×10^{-3}	78 (44)

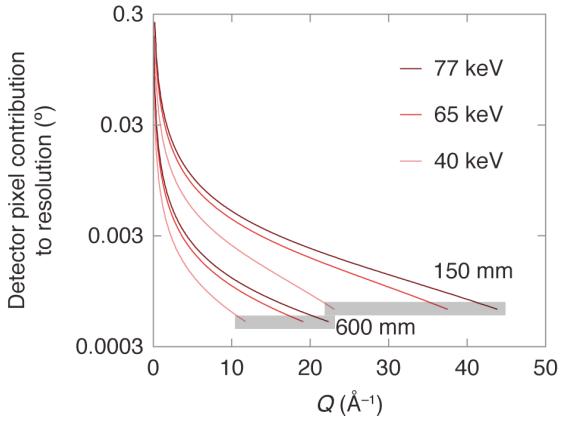
As this table anticipates, the design concept of XPDF is to use three different monochromator crystal cuts—each operating at the same fixed beam geometry—in order to select three different energies for PDF measurements. Changes between operating energies will be minimally disruptive to operations since they can be achieved through straightforward translation of a carousel that houses three appropriately-cut silicon crystals. By adopting a fixed monochromator configuration, the sample point remains fixed and consequently allows for highly optimised design of post-monochromator beam collimation, shielding for high energy parasitic background scattering and

sample-detector configurations. In addition, by adopting a double crystal monochromator design it will be possible to reduce harmonic contamination of the X-ray beam by slight detuning of the parallelism between the two crystals. The Q_{max} values obtained are well suited to PDF studies. In the table the theoretical maximum values ($2\theta = 180^{o}$) are given together with (in parentheses) the values that are expected for routine operation when using a 2D detector as described below. So, for example, the (220) configuration offers a theoretical Q_{max} of 66 Å^{-1} but in the standard operation mode will be used to collect data to Q_{max} = 38 Å^{-1}. We note that these operating values are similar to those offered at the APS X-ray PDF beamline 11-ID-B.

Two classes of detector are required to maximise the flexibility of the station for the envisaged science programme:

1. One or more flat panel amorphous silicon detectors equipped with CsI scintillators are expected to be the primary detector configuration. These devices are typically pixellated at the 2000 × 2000 pixel level, with a pixel pitch of 200 μm. Their resolution and maximum Q-range is determined by the distance between the detector and the sample. It is envisaged that the sample table will allow this distance to be controlled by driving the detector module back and forth along the beam axis. Access to multiple sample-to-detector configurations allows judicious balancing of Q_{max} and ΔQ depending on the scattering behaviour of individual samples and the particular science question to be addressed. This type of detector is also ideally suited to time-resolved studies, since they can generally be operated at a frame rate in excess of 30 Hz.

2. The second detector option would be the use of a 1D strip detector that covers a large 2θ range to access the higher Q region, whilst also delivering a high frame rate suitable for time-resolved PDF measurements. Currently no detector of this type is available for high energy operations (>30 keV), but a number of developments are currently in progress at various institutions and companies.

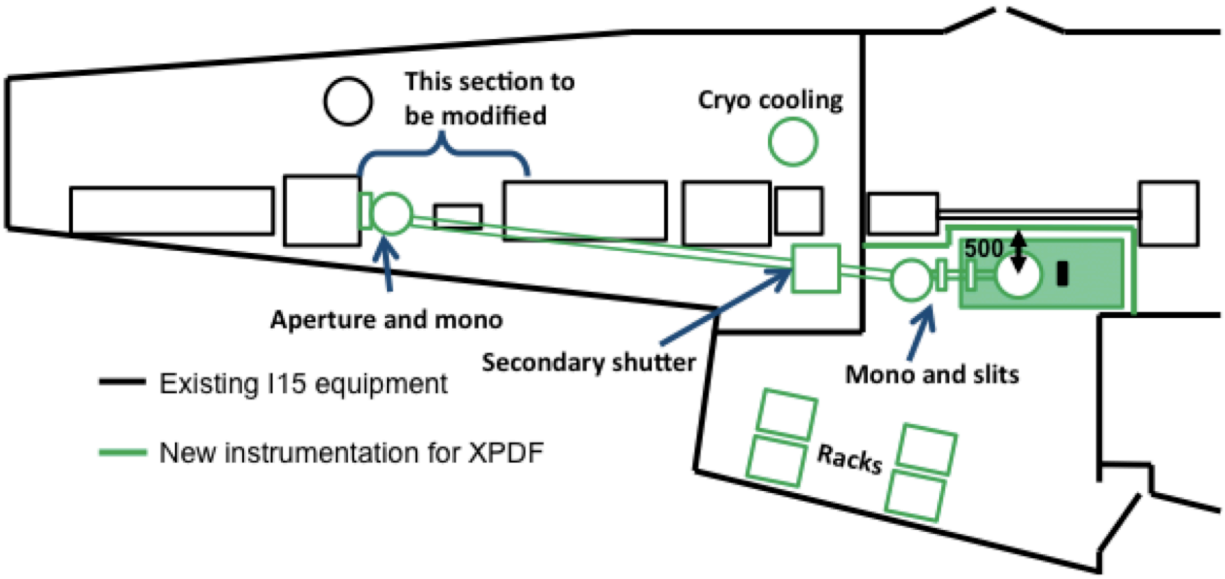


Detector contribution—free of sample size or beam size effects—to the angular resolution as a function of Q for the three proposed X-ray energies and with a 400 mm detector with 200 μm pixels placed at 150 mm and 600 mm from the sample. This graph also shows the maximum value of Q that can be obtained for each configuration.

The figure shows the expected performance of a flat panel detector as a function of sample–detector distance, and for the beam characteristics proposed for XPDF. At the shortest distance (150 mm) and highest energy (76 keV) the angular resolution of the device is sufficient to separate the Bragg scattering features from a crystal with a cell volume of 1000 Å^3, whilst delivering a potential real space resolution in the PDF of 0.07 Å. At a longer distance of 600 mm and the same energy the angular resolution is improved to allow the Bragg scattering to be resolved from a crystal with a unit cell volume of 8000 Å^3, but the real space resolution of the PDF is reduced to 0.14 Å. If ever required, still greater Bragg peak separation can be obtained by measuring with lower X-ray energies.

4. Beamline Specification

Perhaps the greatest challenge in designing XPDF has been to construct an optimal PDF beamline whilst minimising the impact on the activities of the existing and fully operational main branch of I15. Shown below is the proposed schematic layout of the side station based on the monochromator configuration discussed above.



A key design (and cost) advantage of our proposal is that XPDF would require construction only of a single lead wall within the existing I15 second optics hutch. This should minimise disruption to the operation of the main branch of the beamline caused by general building infra-structure work. The fixed take-off geometry monochromator is necessarily a cryo-cooled device due to the high radiation power delivery of the wiggler source. The two crystal reflections are separated between the first optics hutch and the XPDF experimental hutch, to provide sufficient separation (*ca* 600 mm) of the side station beam from the direct beam delivered to the main branch of the beamline. An additional beam shutter in the first optics hutch will allow independent operation of the side station provided the main I15 port shutter is open.

The sample point is conveniently positioned above an optical table that has surface dimensions of 1 m × 2.25 m. This is sufficiently large to allow all detectors and goniometers to be mounted on the sample table. The sample position is 36 m from the wiggler source which results in a maximum beam size at the sample position of 3.6 mm × 3.6 mm, assuming the adoption of the proposed 100 µrad × 100 µrad primary beam collimator. The photograph to the right is of the existing I15 second optics hutch and shows the area that would be converted

into the XPDF sample hutch. The experimental table that would hold the sample position and the detectors and goniometers would occupy the space to the right of the I15 main beam transport tube, in front of the personnel barrier visible in the centre of the photograph (see marked footprint). User access to the XPDF experimental hutch would be from an existing door to the right of the photograph (not visible).

The default beam size corresponds to a photon flux density on the sample position of 10^{10}–10^{11} photons/s.mm^2 and in some instances it may be desirable to enhance this through beam focussing. Given the simple optical layout of XPDF and the high energy of the photon beams, we propose to install a series of compound refractive lenses between the two monochromator crystals that may be automatically inserted into the beam to avoid interrupting I15 operation. This unit will allow us to focus the beam at the sample position if higher flux density is required for a specific experiment.

To conclude the discussion of the beamline configuration it is necessary to note the expected configurations of the sample point. It is anticipated that the most frequently requested sample geometry will be a spinning capillary mounted on the θ circle. This rotation stage would also allow for mounting flat plate geometry samples. In addition to the rotation stage and to allow maximum versatility in the use of the flat panel detector (detector option (1) above) and range of samples that can be studied, we also intend that the XPDF experimental table is equipped with a high precision X-Y-Z-φ-ψ-χ stack of motorised stages.

Sample environments

The growing worldwide interest in the X-ray PDF technique has already led to the development of a wide range of highly compact advanced sample environment equipment that will be suitable for installation at XPDF. Examples include gas flow reactors for *in situ* catalysis that have been developed at 11-ID-B of the Advanced Photon Source, and multi-probe cells, that combine optical (IR/Raman) and X-ray techniques that are under development at the European Synchrotron Radiation Facility. It is anticipated that XPDF will be able to capitalise on many of these developments, although for initial-phase operations we would intend only that the beamline be equipped with a basic suite of sample environment equipment: a helium cryostat, a cryostream cooler, a resistive element furnace and a sample-changer for high-throughput measurements. Beyond this, the fixed beamline geometry and flexible sample stage setup should facilitate the development and installation of a wide range of as-yet-unspecified sample environments. Installations such as flow cells, electrochemical cells, applied fields cells or large volume pressure cells are all easily envisaged as upgrades. Possible sample environments of greater technical complexity include mirror furnaces, levitators, laser heating and spectroscopic equipment for simultaneous PDF+IR/Raman measurements.

Expected impact on the existing beamline, I15

Once installed, XPDF is designed to operate independently of the main branch of I15, apart from the need to share the main port shutter of the insertion device. One of the key aims of the proposed technical design was to minimise the extent of disruption to operation of I15, both in terms of the degree of construction work required for the assembly of new radiation enclosures and cabins, and also with respect to the scale of any modifications required for the performance of critical existing beamline components, such as monochromator and mirrors. Where possible we have taken advan-

tage of existing design features of I15 that were originally incorporated to allow for the future construction of monochromatic or white beam side stations. It is worth noting that the original design plan for I15 itself anticipated the construction of a side-station.

Implementation of the proposed XPDF design is expected to require the following modifications to I15:

1. The major construction work will be the creation of the XPDF experimental area within the second optics hutch of I15. Taking advantage of the existing structure means that the proposed design will only require the erection of a single lead partition wall of 5 cm thickness. During this period a beam exit path will also be cut in the back wall of the first optics hutch. In total it is anticipated that this work will require a three month shutdown period to allow for the construction of the partition wall and for the re-routing and installation of the various electrical and fluid services in the newly-separated radiation enclosures. If this period is scheduled to coincide with a standard period of shutdown at Diamond (one month), then the impact on the I15 operating cycle is minimised to a two month interruption in service together with an additional month for re-commissioning.
2. Equipment located before the I15 monochromator will need some modifications and redesigning: although the side beams come into the first hutch, they are immediately stopped by a mask. The placement of the first aperture and monochromator vessel of XPDF is immediately after the monochromator of the main branch of I15. This space is occupied by a beam diagnostic unit and white beam mask, both of which will need to be redesigned and repositioned.
3. The exit beam of the first monochromator vessel of XPDF is angled away from the main beam of I15, towards the synchrotron. The take-off angle of 5.68° required to obtain high energy photons means that the beam will transect an Oxford instruments viewer used for viewing the main beam of I15 on leaving its monochromator. This device will have to be modified or removed to allow the XPDF beam to pass.
4. The next vessel in the first optics hutch is a mirror box for the main branch of the beamline. In anticipation of future side stations, this vessel has already been shaped during the original I15 build to allow a side-station beam to pass.
5. The final major elements of XPDF within the first optics hutch are the compound refractive lenses and the beam shutter. These devices should not require any modifications to main branch components, and the latter will permit the XPDF experimental hutch to operate independently. Assuming that the main optical components for XPDF can be assembled and tested off-line, the installation of the side-station should be entirely feasible within planned shutdown periods in the Diamond operating schedule. The modifications to the beam diagnostic elements of the main branch of I15 may require a small amount of re-commissioning work to be performed on that instrument, but no major optical re-alignments are anticipated.

In summary, allowing for a short commissioning period for the optical elements of XPDF in the shared first optics hutch, the development of this side station should not interrupt normal service from the main branch of the beamline for more than four months.

5. Costs

Category	Budget (£k)
Insertion Device and Straight Section	
Front end	
Modifications to main I15 instrumentation	
Hutch modifications	
Cabin and Services Modules	
Two side bounce liquid-nitrogen cooled monochromators	
Slits	
Absorber, collimators and shutter	
Convex refractive lenses	
Diagnostics	
Sample table	
Sample x,y and goniometer stage	
Sample environment stages	
I0 detector	
Perkin Elmer 2D detectors	
Vacuum pumps, bellows, gauges	
Computing	
Racks	
Vacuum controls	
Motion controls	
Diagnostic controls	
Cables	
PSS	
Miscellaneous	
Total	

6. Call for Expressions of Interest

"*A beamline is proposed that measures X-ray pair distribution function (PDF) data of the highest quality possible at DLS, servicing the very large number of UK research groups whose work relies on understanding local structure in materials. These research areas span all the key priority themes of materials development: energy (battery materials, carbon capture via gas sorption, hydrogen storage, catalysts); health pharmaceuticals, (biomaterials); digital economy (digital storage media, electronics materials and semiconductor components, display materials, plastic electronics).*

"The User Working Group are preparing the joint full proposal. We are inviting users to submit letters of support detailing why they are supporting the proposal and what research they would carry out on the beamline if it is recommended for construction. Letters of support of no more than 2 A4 pages.

"Letters of support for the beamline need to be submitted to Andrew Goodwin, chair of the user working group, by extended deadline 20th January 2011."

7. Expressions of Interest Table

Letters of support for XPDF (appended) were received from the following individuals.

Industry (8)

Dr Anne Kavanagh	AstraZeneca
Dr Peter Timmins	Bristol-Myers Squibb
Dr Matthew Johnson	GSK
Dr Tim Hyde	Johnson Matthey
Dr Brett Cooper	Merck
Dr Cheryl Doherty	Pfizer
Dr Neil Feeder	Pfizer
Dr Su Varma	Pilkington

Central Facilities (13)

Dr Kirsten Christensen	I19	DLS
Dr Adrian Hill	ID-31	ESRF
Dr Emma Barney	Disordered Materials	ISIS/RAL
Dr Daniel Bowron	Disordered Materials	ISIS/RAL
Dr Samantha Callear	Crystallography	ISIS/RAL
Prof. Felix Fernandez-Alonso	Molecular Spectroscopy	ISIS/RAL
Prof. Alex Hannon	Disordered Materials	ISIS/RAL
Prof. Stephen Hull	Crystallography	ISIS/RAL
Prof. David Keen	Crystallography	ISIS/RAL
Prof. Robert McGreevy	Diffraction & Muon Division	ISIS/RAL
Prof. Alan Soper	Disordered Materials	ISIS/RAL
Dr Matthew Tucker	Crystallography	ISIS/RAL
Dr Jeppe Christensen	I711	MAX-lab, Lund

Academia (56)

Prof. Neville Greaves	Mathematics and Physics	Aberystwyth
Dr Martin Wilding	Mathematics and Physics	Aberystwyth
Dr Richard Martin	Life and Health Sciences	Aston
Dr Andrew Burrows	Chemistry	Bath
Prof. Philip Salmon	Physics	Bath
Dr. Joseph Hriljac	Chemistry	Birmingham
Dr Adrian Barnes	Physics	Bristol
Prof. Jacqui Cole	Physics	Cambridge
Prof. Martin Dove	Earth Sciences	Cambridge
Prof. Stephen Elliott	Chemistry	Cambridge
Prof. Lindsay Greer	Materials Science	Cambridge
Prof. Clare Grey	Chemistry	Cambridge
Prof. Simon Redfern	Earth Sciences	Cambridge
Prof. Kenneth Harris	Chemistry	Cardiff
Prof. John Evans	Chemistry	Durham
Dr Ivana Radosavljevic Evans	Chemistry	Durham
Dr Christoph Salzmann	Chemistry	Durham
Dr Stephen Moggach	Chemistry	Edinburgh
Prof. Simon Parsons	Chemistry	Edinburgh
Dr Ian MacLaren	Physics and Astronomy	Glasgow
Dr Stephen Skinner	Materials	Imperial
Dr Serena Corr	Physical Sciences	Kent
Dr Gavin Mountjoy	Physical Sciences	Kent
Prof. Bob Newport	Physical Sciences	Kent
Dr John Claridge	Chemistry	Liverpool
Dr Yaroslav Khimyak	Chemistry	Liverpool
Prof. Matthew Rosseinsky FRS	Chemistry	Liverpool
Prof. Robert Jones	Chemistry	Nottingham
Dr Simon Clarke	Chemistry	Oxford
Prof. Peter Edwards FRS	Chemistry	Oxford
Dr Michael Hayward	Chemistry	Oxford
Prof. Chris Hardacre	Chemistry & Chemical Engineering	Queen's University Belfast
Dr Ann Chippindale	Chemistry	Reading
Dr Simon Hibble	Chemistry	Reading
Dr Kenneth Shankland	Pharmacy	Reading
Prof. Keith Ross	Physics	Salford
Prof. Lee Brammer	Chemistry	Sheffield
Prof. Mike Gibbs	Materials Science & Engineering	Sheffield
Dr Russell Hand	Materials Science & Engineering	Sheffield
Prof. Neil Hyatt	Materials Science & Engineering	Sheffield
Dr Michael Ojovan	Materials Science & Engineering	Sheffield

Prof. Ian Reaney	Materials Science & Engineering	Sheffield
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Prof. Gopinathan Sankar	Chemistry	UCL
Prof. Neal Skipper	Physics	UCL
Dr Diane Holland	Physics	Warwick
Prof. Tim Jones	Chemistry	Warwick
Dr Dean Keeble	Physics	Warwick
Prof. Pam Thomas	Physics	Warwick
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